Group Contribution+ (GC+) Based Estimation of Environment-Related Properties for Design of Sustainable Processes: Development of Property Models and Uncertainty Analysis

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Currently there is a great deal of interest in the development of methods and tools for the process synthesis, design, and analysis of sustainable processes. The design of sustainable processes require that it should satisfy various conditions (or constraints) such as, increased productivity, minimum energy consumption, reduction in raw materials, recovery of products, minimum generation of pollution etc. (Carvalho et al., 2006). This task can be performed by using a chemical process simulator (to perform mass and energy balance for the concerned process) together with the waste reduction (WAR) algorithm (Young and Cabezas, 1999) to obtain a quantitative measure of the potential environmental impacts which, as part of LCA analysis of process synthesis and design, contributes to identify sustainable processing paths and design alternatives. The basis for the quantification of the environmental impacts is a set of environment-related properties (such as, fathead minnow LC50 (96-hr), oral rat LD50, global warming potential etc.) of chemical substances involved in the process. For many chemicals of interest the experimental data of environment-related properties is not available since the measurement of these properties are extremely time consuming and expensive. Also, processes that deal with synthesis of new chemicals require a suitable property prediction method in order to obtain reliable estimates of environment-related properties of new chemicals. In such cases, group contribution (GC) methods are generally suitable to obtain the needed property values since these methods provide the advantage of quick estimates without requiring substantial computational work. In GC methods, the property of a chemical is a function of structurally dependent parameters which are determined as a function of the frequency of the groups representing the chemical and their contributions. Among the GC methods for estimation of properties of chemicals, the Marrero and Gani (MG) method (Marrero and Gani, 2001) is well-known. The MG method allows estimation of properties based exclusively on the molecular structure of the chemical and exhibits a good accuracy and a wide range of applicability covering chemical, biochemical, and environment-related chemicals. For the case where the molecular structure of a given chemical is not completely described by any of the available groups, the atom connectivity index (CI) method has been employed together with MG method to create the missing groups and to predict their contributions (Gani et al., 2005). This combined approach has led to the development of group contribution^{+} (GC^{+}) method of a wider application range than before since the missing groups and their contributions can now be easily predicted through the regressed contributions of connectivity indices. In addition to the accuracy of predicted property values, it is also important to know the uncertainties of the estimated property values that arise due to uncertainties in the regressed parameters of the selected property model.

The main objective of this work is to develop property prediction models based on the GC^{+} approach (combined GC method and CI method) to provide reliable estimates of environment-related properties together with uncertainties (for example, prediction error in terms of 95% confidence interval) of the estimated property values. For this purpose, a systematic methodology for property modeling and uncertainty analysis developed by Hukkerikar et al. (2012) is used. The methodology includes a parameter estimation step to determine parameters (group/atom contributions, adjustable parameters, and a universal parameter) of property models, and an uncertainty analysis step to establish statistical information about the quality of parameter estimation, such as the parameter covariance, the standard errors in predicted properties, and the confidence intervals. For property modeling with a GC method, the MG method has been considered. For property modeling with a CI method, the models proposed by Gani et al. (2005) have been considered. For parameter estimation, large data-sets of experimentally measured property values of wide range of chemicals (hydrocarbons, oxygenated chemicals, nitrogenated chemicals, poly-functional chemicals, etc.) taken from the database of US Environmental Protection Agency (EPA) is used. In total 10 environment-related properties, which include the fathead minnow LC50 (96-hr), *daphnia magna* LC50 (48-hr), oral rat LD50, aqueous solubility, bioconcentration factor, permissible exposure limit (OSHA-TWA), photochemical oxidation potential, global warming potential, ozone depletion potential, and acidification potential have been modeled and analysed. The application of the developed property models for estimation of environment-related properties and uncertainties of the estimated property values is highlighted through several illustrative examples. The developed models for environment-related properties have been implemented in ProPred, a property estimation toolbox of ICAS ® (Integrated Computer Aided System) software developed by CAPEC, DTU. The developed property models provide reliable estimates of environment-related properties needed to perform design and analysis of sustainable processes and allow one to evaluate the effect of uncertainties of estimated property values on the calculated PEI index of the process giving useful insights into quality and reliability of the design of sustainable processes. The use of the developed property models for environment-related properties in the design of sustainable process is highlighted through a case study.

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